

## CONCERNING THE FERMI SURFACE OF TIN

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The dimensions of extremal electron orbits in the (001) plane are studied by the size effect method. The results are compared with the nearly-free-electron model.

IN a previous paper,<sup>[1]</sup> the size effect was used in measurements of the surface impedance at radio frequencies to study the Fermi surface of tin. The dimensions of the extremal orbits were measured, orbits that arise in those cases in which the magnetic field lies in one of the two crystallographic planes: (100) or (110). It was found that as applied to tin, which has several extremal orbits for each direction of the magnetic field, which furthermore contribute to the conductivity, the size effect method is more productive than the other known methods. Therefore, the study of the size effect in tin was extended this time to a specimen with a surface normal  $n \parallel [001]$ , i.e., when the magnetic field lying in the plane of the specimen is located in the (001) plane—the third of the principal crystallographic planes.

In this case, a number of new data were obtained which could be used for establishing the shape of the Fermi surface. These data are presented in the present article.

## EXPERIMENT

The measurements were carried out with the apparatus described in<sup>[1]</sup>. The dependence of the frequency  $f$  of a vacuum oscillator on the magnetic field  $H$  is measured by the modulation method. The specimen is put in the coil of the tank circuit of the oscillator. In this way, the field dependence of the imaginary part  $X$  of the surface impedance of this specimen is determined. The specimens had the shape of disks of diameter 18 mm and thickness  $d = 0.4$  mm for one and  $d = 0.6$  mm for the other. The angle between the normal to the surface of the disk and the [001] axis amounted to  $45'$  for the first specimen, and  $30'$  for the other. The specimens were cast in a dismountable quartz form<sup>[2]</sup> out of metal which contained about  $10^{-4}$  per cent impurity.

The results of measurement of the dimensions of the extremal cross sections in the (001) plane are shown in the polar diagram of Fig. 1. The radius in this diagram denotes the value of the

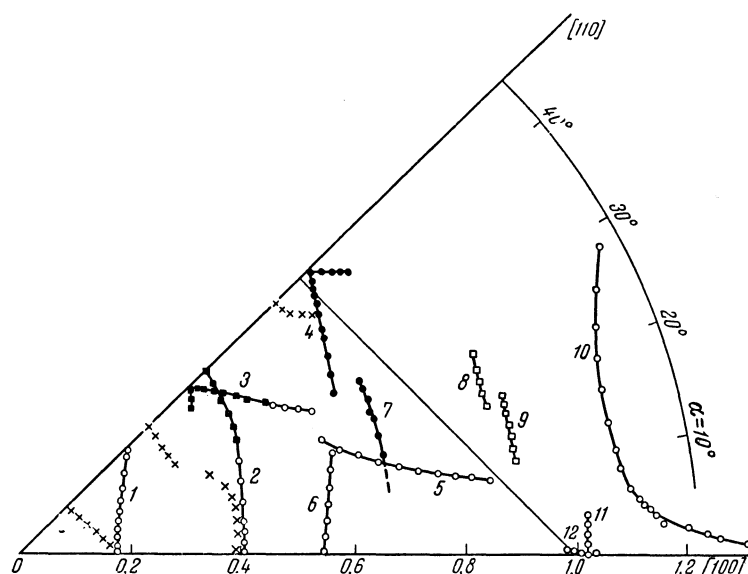


FIG. 1. Anisotropy of the half-width of the extremal orbits in the (001) plane. The various types of lines are denoted by the different symbols (see<sup>[1]</sup>, Figs. 6-8). The crosses denote data from ultrasonic measurements;<sup>[3]</sup> the thin lines denote the central cross section of the Brillouin zone;  $\alpha$  is the angle between the direction in which the momentum is measured and the [100] axis.

extremal momentum  $p$ , determined from the formula  $2p = edH/c$  (see [1]) in units of  $p_0 = 2\pi\hbar/a = 11.4 \times 10^{-20}$  g-cm/sec. For convenience in further reference, all the so-called "cross sections" are numbered.

As in the case of the (100) and (110) planes, the line intensities, which are given by the different extremal cross sections, differ by about two orders of magnitude. The most intense lines of the cross section 10 are in the range of angle  $10^\circ < \alpha < 28^\circ$  for transverse polarization, that is, for  $E \parallel [100]$  (the line of cross section 10 at  $\alpha < 10^\circ$ , and also the cross sections 5 and 12 were seen only for longitudinal polarization, in which  $E \parallel [010]$  makes a small angle with  $H$ , and for intermediate polarization,  $E \parallel [110]$ ). Some of the intense lines on the curves have long, oscillatory tails (see Fig. 2), the shape of which does not change with change in the thickness of the specimen, frequency, inclination of the field, etc. In all probability, such a strongly non-monotonic dependence of  $\partial X/\partial H$  on  $H$  is connected with the appearance of "chains" of two links: [4, 5] an extremal orbit which produces the line itself, and some sort of extremal orbits of small dimensions. The size effect for such small orbits is observed directly only on the cross section 1; however, it must be kept in mind that the observation is made

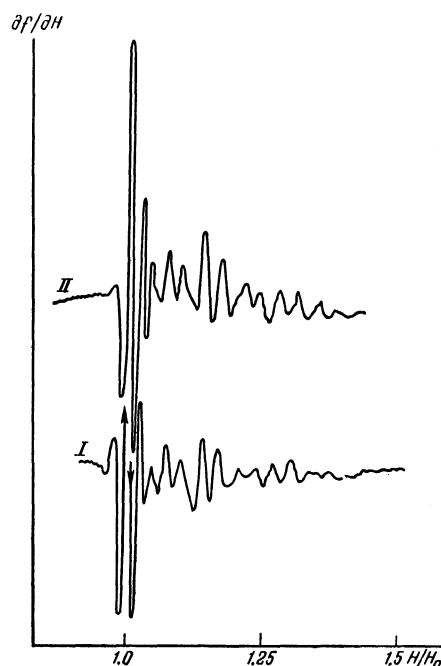


FIG. 2. Recorded lines of the size effect for  $n \parallel [001]$ ,  $E \parallel [100]$ .  $H$  lies in the plane of the specimen and makes an angle of  $14^\circ$  with the  $[010]$  axis (the cross section 10); curve I —  $d = 0.4$  mm,  $T = 2.2^\circ\text{K}$ ,  $f = 3.3$  Mc; II —  $d = 0.6$  mm,  $T = 3^\circ\text{K}$ ,  $f = 3.7$  Mc. The record of the very high maximum is cut off on curve I.

much more difficult for small fields by superconductivity (it becomes necessary to work at  $T > 3.7^\circ\text{K}$ ) and by the strong monotonic dependence of the impedance on the field, against the noise background of which it is difficult to observe the desired signal. The fact that the tails after the various lines are very similar for a fixed direction of the field, with the same distances between extrema, supports the explanation just given.

## DISCUSSION

We now proceed to the identification of the cross sections used. Here, as earlier, we shall start out from the nearly free electron model. According to this model, there are in tin [6] three open surfaces in zones 3, 4a and 5, and also several closed surfaces in zones 2, 4b, 5 and 6. The most accurate calculation by the OPW (orthogonalized plane wave) method shows [7] that the second zone is completely filled.

Four of the groups of lines in the diagram—the "cross sections" 3, 4, 11 and 12—are connected with open trajectories. [8] Here, the presence of the lines 3 gives testimony of the unusual complexity and the broken nature of the corresponding open orbits in momentum space. The fact that the lines 3, 4 and 12 split off and are displaced when the magnetic field is inclined relative to the surface of the specimen [which means, relative to the crystallographic planes (001), which is more significant] demonstrates this broken character. In this connection, we recall that the size effect allows us to measure the projection of the distance between the points of contact in the direction determined by the vector derivative normal to the surface and to the vector magnetic field. For orbits that are sufficiently simple in shape, the location of the points of contact on the Fermi surface does not change with change in the angle of inclination  $\varphi$ . In this case the shift of the lines could come about only because of the change in the effective thickness of the plate—a replacement of  $d$  by  $d/\cos \varphi$  which, for small  $\varphi$ , is quite unimportant. Experiment has shown that, for all cross sections except 3, 4 and 12, the location of the lines does not depend on the angle of inclination (for most lines, we have verified this circumstance up to angles  $\varphi \sim 5^\circ$ .)

The cross sections 6 and 10 pertain to the open surfaces in the fourth zone, which appears in the best way in all the experiments on tin. As a whole, the results of the study of this surface by the size effect method are summarized in qualitative fashion in Fig. 3. All possible types of orbits have

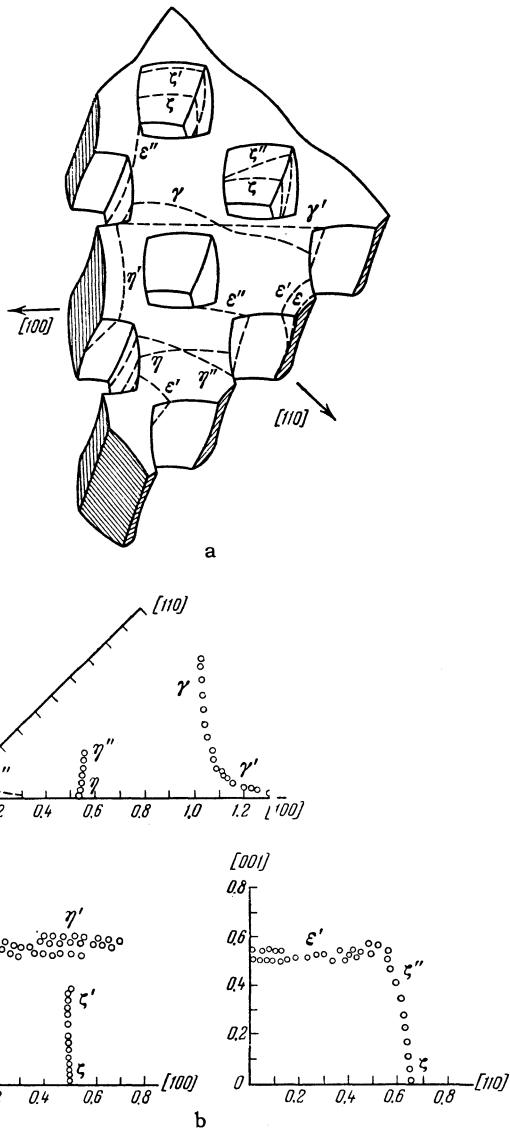


FIG. 3. a - Simplified model of the Fermi surface of the 4a zone (the shaded region is not filled with electrons), b - is the cross section determined by the size effects on the extremal orbits of this zone.

been observed experimentally, with the exception of the orbits  $\epsilon''$  on specimens with  $n \parallel [001]$ . (The cross section which should have been obtained for the orbits  $\epsilon''$  is shown in Fig. 3b by the dotted line. It is constructed from the experimental points of cross section 10.) It is interesting to note that, in the (001) plane, a very intensive size effect is observed from the so-called "elongated" orbits, which encompass two unit cells of the reciprocal space—the orbits  $\gamma$  and  $\gamma'$ , cross section 10. Data on the degree of quantitative agreement of the results of the experiment with the nearly free electron model for the zone 4a are given in [1] and [9].

The cross section 2 is "joined together" on the [100] and [110] axes with the cross sections

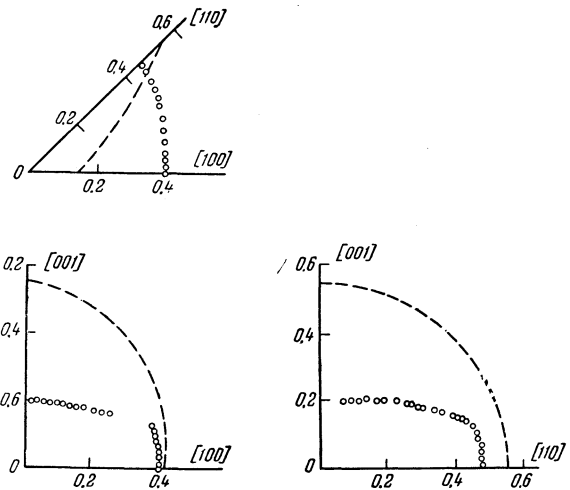


FIG. 4. Dimensions and shape of the closed Fermi surface in tin as determined by the size effect. The dashed line indicates the almost free electron model.

$3_1$  and  $3_2$  from [1]. Taken together, they determine the closed surface (Fig. 4). It should probably be compared with the surfaces of the zone 4b of the model, although, as already pointed out, it no longer has the characteristic cross-shaped form when projected on the (001) plane.

Thus, a rather unique situation arises. The surfaces of zones 3 and 4a follow the model of almost free electrons very well, with accuracy to several per cent of the period of the reciprocal lattice. [1] The surface of the zone 4b differs very strongly from the model; it is, as it were, contracted by the forces of surface attraction with the volume remaining constant. The reasons for such a difference between the surfaces is quite unclear. It seems to us that this process deserves a theoretical investigation.

No lines which should be obtainable from the extremal orbits of zone 3 were observed in the weak fields. All the other cross sections are apparently connected with the surface of zone 5.

As a whole, the results obtained can be summarized in the following way. It has been established that there are in tin: an open surface, very similar to the almost free electron model (zone 4a); a closed surface, whose dimensions provide a basis for assuming it to correspond to the surface of zone 4b of the model; a surface corresponding to zone 3 of the model, which is apparently closed; [1] a complicated open surface corresponding to zone 5 of the model, the detailed structure of which has not yet been worked out. [1]

Nothing definite can be said concerning zones 2, 6 and the closed part of zone 5.

However, the question arises as to how unique are the resultant conclusions; does not the abund-

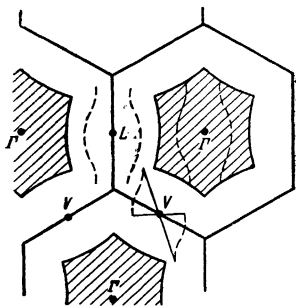


FIG. 5. Possible locations of the orbits  $4_1$  in the intersection of the reciprocal lattice with the (100) plane which passes through the center of the Brillouin zone. The shaded cross sections are those of the 4a zones in the almost free electron model.

ance of experimental cross sections give an unlimited number of possibilities for comparison with any model? We shall present some arguments that demonstrate the degree of probability of the other interpretations.

We begin with the assumption that the existence of an open surface of zone 4a has been proved. Then the principle of the non-crossing of the Fermi surface<sup>[10]</sup> immediately reduces the number of available possibilities. (The symmetry of tin admits only the presence of isolated points of degeneracy on the  $C_4$  axis; this possibility is apparently not realized.) The surface of zone 4a divides the Brillouin zone into two parts. Every other surface should be located as a whole either in an external or an internal part. According to the nearly free electron model, the surfaces of zones 3 and 4b are inside the zone 4a (i.e., in the region not occupied by the electrons), while the surface of zone 5 is on the outside—between the layers of the surfaces of zones 4a. We now select one of the unidentified cross sections in the (100) planes—the cross section  $4_1$ . It is connected with the largest orbits and has a characteristic shape. We assume that it is located in zone 5. One such possibility is demonstrated in Fig. 5—the cross section  $4_1$ , which is located in the vicinity of the point V. In principle, however, other variants are possible.

The cross section  $4_1$  can be located inside the surface 4a in only one way: by making the point  $\Gamma$  the center of the orbits. This would mean that the cross section  $4_1$  belongs to the fourth zone. The surfaces 4a and 4b would be joined in a single complicated surface—an additional set of tubes along the axis  $C_4$  ([001]) would appear on the open surface. Then the surface  $(3_1, 5_1, 3_2, 2)$  would have to be transferred from the region about the point  $\Gamma$  to another place, for example, to the region around the point L. Although this would

not seriously contradict the experimental points in Fig. 3 [the orbits  $\eta'$  and  $\eta''$  for the magnetic field in the (001) plane can be noncentral], but there is no experimental confirmation of the existence of such a surface. In particular, additional cross sections in the (001) plane should appear.

In the second variant, the center of the orbits of the cross section  $4_1$  are located at the point L. The cross section should then pertain to the surface of the zone 5. According to the nearly free electron model, the surface of zone 5 is the boundary of the volume of p space, which is infinitely extended in the (001) plane: this is in fact a stratified set of surfaces, each of which is strongly cut up, curved, etc. Placing the cross section  $4_1$  close to the point L, we then introduce the vertical crosspieces between the layers, located in checkerboard fashion. The surface becomes infinitely extended also in the [001] direction. This in itself does not contradict the data of Alekseevskiĭ and Gaĭdukov<sup>[11]</sup> on the presence of orbits closed in the [001] direction. One can visualize such a layered structure for which there should be no such orbits. However, such a structure would be to some degree “accidental”. Therefore, we shall assume that, in actuality, the cross section  $4_1$  pertains to the fifth zone and is located somewhere in the layer between the 4a surfaces.

Thus, the existence of data on the extremal orbits in the three principal crystallographic planes has been shown to be inadequate for the complete reconstruction of the entire Fermi surface. The next step should be the study of a series of specimens with intermediate orientations. However, the expediency of a detailed study at the present time, before the appearance of some sort of special theoretical interest in the given area, appears to be doubtful.

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